Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:19 PM GMT

PDB ID	:	3WTT
Title	:	Crystal structure of the complex comprised of phosphorylated ETS1, RUNX1, CBFBETA, and the tcralpha gene enhancer DNA
Authors	:	Shiina, M.; Hamada, K.; Ogata, K.
Deposited on	:	2014-04-21
Resolution	:	2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

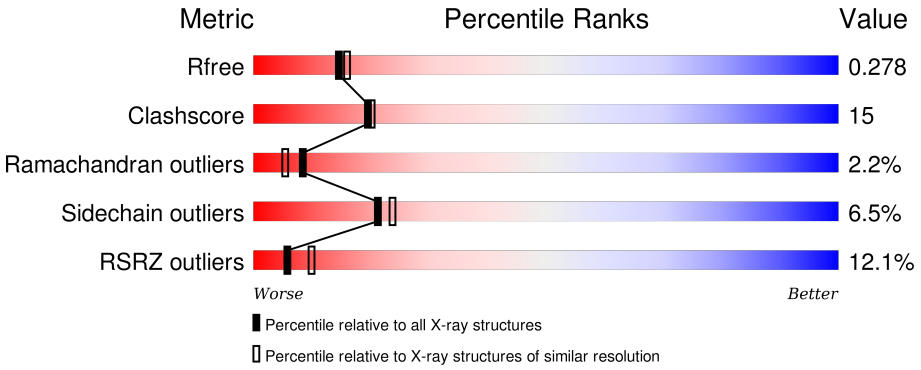
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	204	45% 13% 42%
1	F	204	50% 7% 42%
2	B	142	18% 50% 37% 5% 8%
2	G	142	13% 53% 35% 8%
3	C	166	56% 14% 29%

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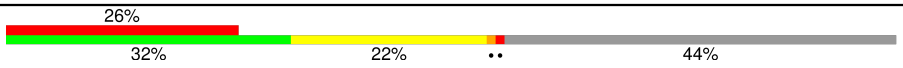
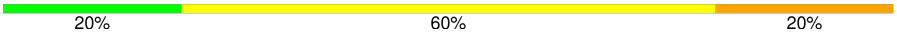
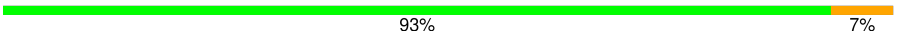
Mol	Chain	Length	Quality of chain
3	H	166	
4	D	15	
4	I	15	
5	E	15	
5	J	15	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7083 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Runt-related transcription factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			919	577	170	168	4			
1	F	118	Total	C	N	O	S	0	0	0
			914	574	169	167	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347
F	94	LYS	LEU	ENGINEERED MUTATION	UNP Q03347

- Molecule 2 is a protein called Core-binding factor subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	131	Total	C	N	O	S	0	0	0
			1078	675	196	201	6			
2	G	130	Total	C	N	O	S	0	0	0
			1071	671	195	199	6			

- Molecule 3 is a protein called Protein C-ets-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	118	Total	C	N	O	S	0	0	0
			967	627	165	171	4			
3	H	93	Total	C	N	O	S	0	0	0
			789	512	137	137	3			

- Molecule 4 is a DNA chain called 5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total 299	C 144	N 54	O 87	P 14	0	0	0
4	I	15	Total 299	C 144	N 54	O 87	P 14	0	0	0

- Molecule 5 is a DNA chain called 5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*C P*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	15	Total 310	C 148	N 59	O 89	P 14	0	0	0
5	J	15	Total 310	C 148	N 59	O 89	P 14	0	0	0

- Molecule 6 is water.

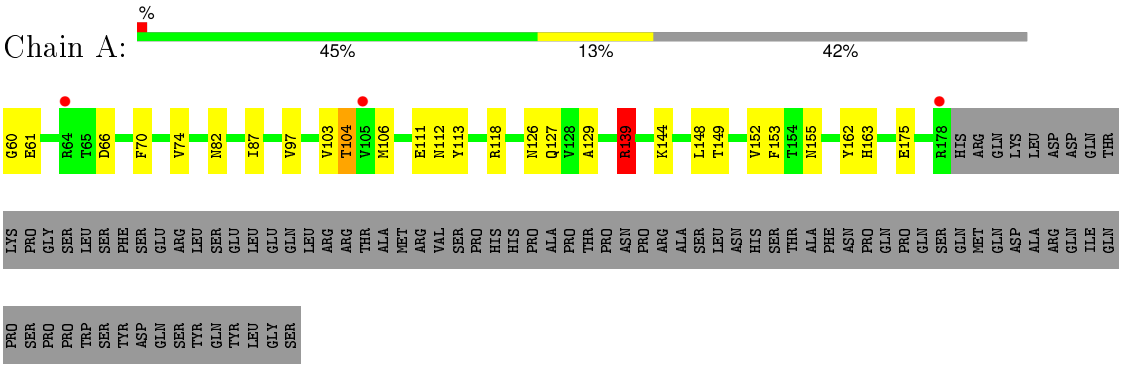
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	19	Total 19	O 19	0	0
6	B	5	Total 5	O 5	0	0
6	C	18	Total 18	O 18	0	0
6	F	24	Total 24	O 24	0	0
6	G	11	Total 11	O 11	0	0
6	H	2	Total 2	O 2	0	0
6	D	9	Total 9	O 9	0	0
6	E	18	Total 18	O 18	0	0
6	I	4	Total 4	O 4	0	0
6	J	17	Total 17	O 17	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

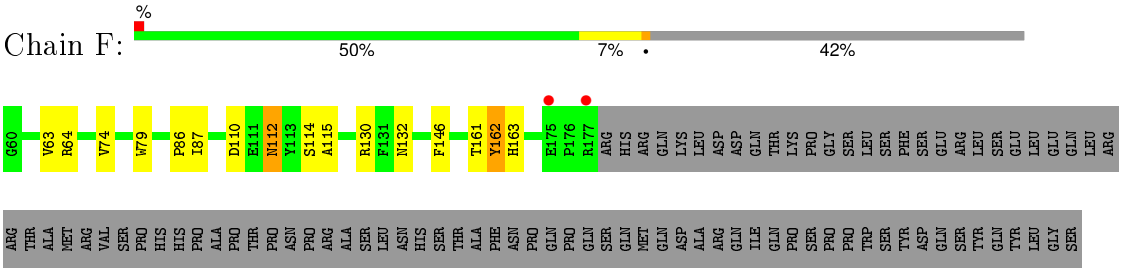
- Molecule 1: Runt-related transcription factor 1

Chain A:



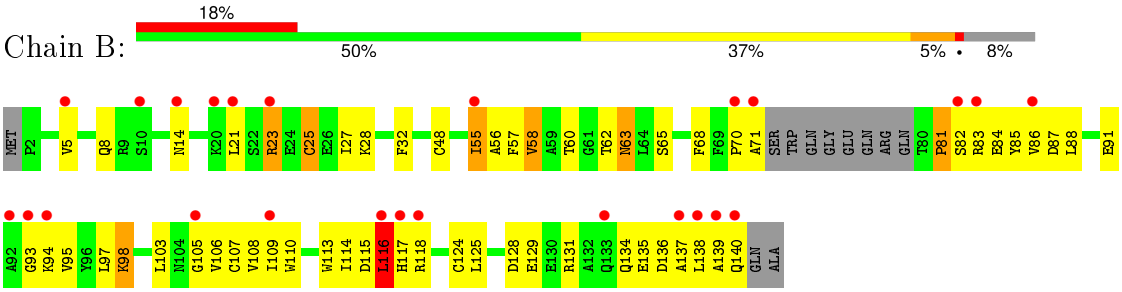
- Molecule 1: Runt-related transcription factor 1

Chain F:



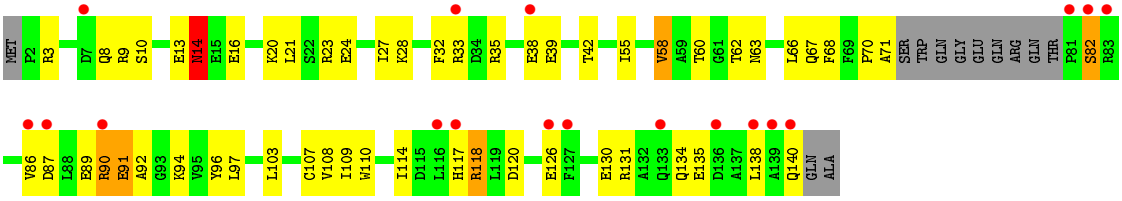
- Molecule 2: Core-binding factor subunit beta

Chain B:

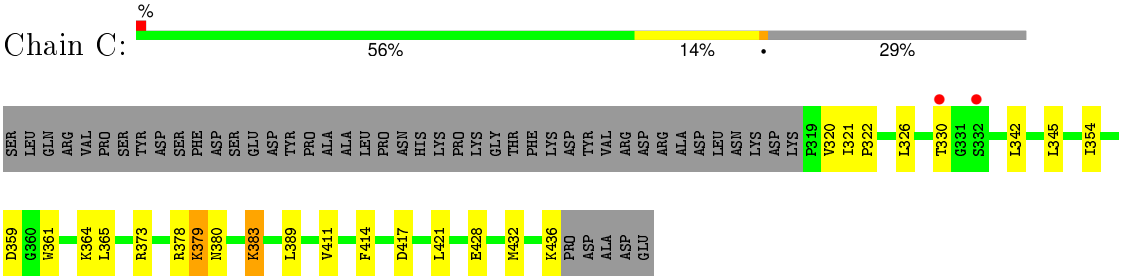


- Molecule 2: Core-binding factor subunit beta

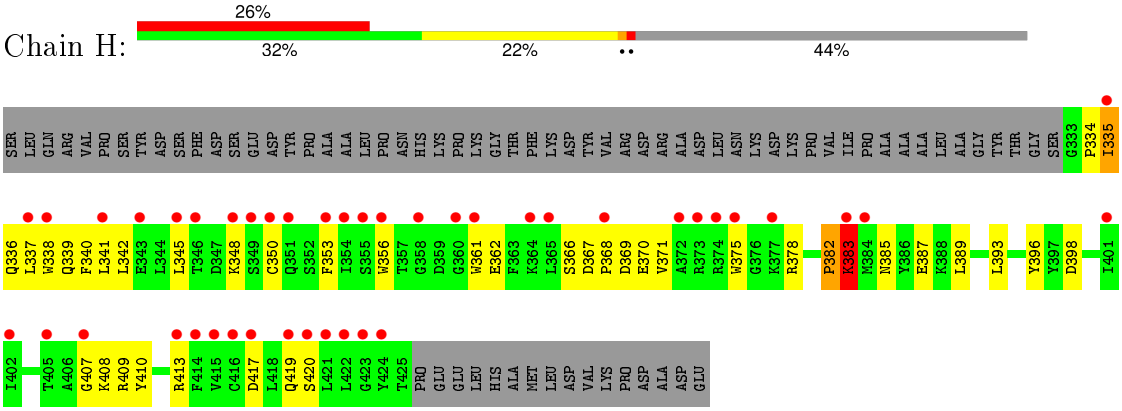
Chain G:



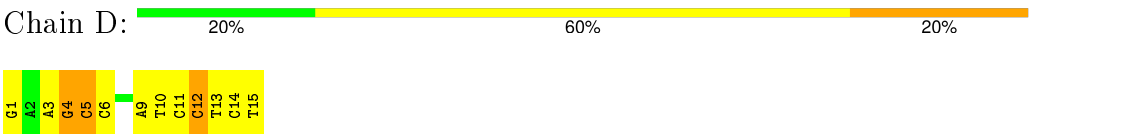
• Molecule 3: Protein C-ets-1



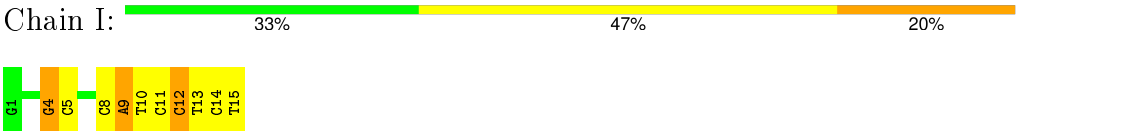
• Molecule 3: Protein C-ets-1



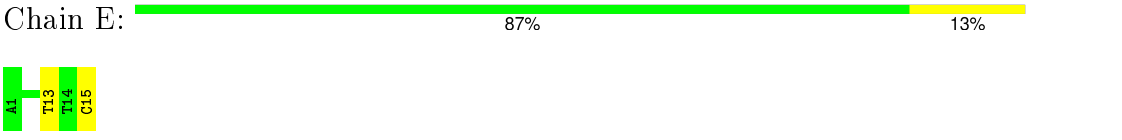
• Molecule 4: 5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3'



• Molecule 4: 5'-D(*GP*AP*AP*GP*CP*CP*AP*CP*AP*TP*CP*CP*TP*CP*T)-3'

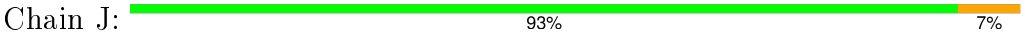


• Molecule 5: 5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3'



• Molecule 5: 5'-D(*AP*GP*AP*GP*GP*AP*TP*GP*TP*GP*GP*CP*TP*TP*C)-3'

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.62Å 101.72Å 194.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.35 48.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.68-2.35) 98.4 (48.68-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.53 (at 2.34Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.241 , 0.277 0.241 , 0.278	Depositor DCC
R_{free} test set	6531 reflections (10.11%)	DCC
Wilson B-factor (Å^2)	65.6	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 64625 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7083	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.64	0/938	0.79	1/1275 (0.1%)
1	F	0.74	0/933	0.88	0/1268
2	B	0.52	0/1100	0.59	0/1477
2	G	0.59	0/1093	0.64	0/1466
3	C	0.71	0/994	0.76	0/1342
3	H	0.45	0/811	0.53	0/1091
4	D	0.92	0/334	1.13	3/512 (0.6%)
4	I	0.85	0/334	1.10	1/512 (0.2%)
5	E	0.87	0/348	0.91	0/537
5	J	0.79	0/348	0.86	1/537 (0.2%)
All	All	0.67	0/7233	0.78	6/10017 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	4
4	I	0	4
5	E	0	1
All	All	0	9

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4	DG	N9-C1'-C2'	-7.67	98.02	112.60
4	I	4	DG	N9-C1'-C2'	-6.95	99.39	112.60
4	D	4	DG	C4'-C3'-O3'	5.56	123.61	109.70
1	A	139	ARG	NE-CZ-NH2	5.29	122.94	120.30
4	D	3	DA	N9-C1'-C2'	5.14	122.38	112.60
5	J	1	DA	OP1-P-O3'	5.14	116.52	105.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	12	DC	Sidechain
4	D	15	DT	Sidechain
4	D	4	DG	Sidechain
4	D	5	DC	Sidechain
5	E	13	DT	Sidechain
4	I	12	DC	Sidechain
4	I	4	DG	Sidechain
4	I	5	DC	Sidechain
4	I	9	DA	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	919	0	924	27	0
1	F	914	0	922	12	0
2	B	1078	0	1040	48	0
2	G	1071	0	1034	42	0
3	C	967	0	966	20	0
3	H	789	0	785	38	0
4	D	299	0	170	15	0
4	I	299	0	170	7	0
5	E	310	0	171	1	0
5	J	310	0	171	1	0
6	A	19	0	0	2	0
6	B	5	0	0	0	0
6	C	18	0	0	0	0
6	D	9	0	0	1	0
6	E	18	0	0	0	0
6	F	24	0	0	1	0
6	G	11	0	0	0	0
6	H	2	0	0	0	0
6	I	4	0	0	0	0
6	J	17	0	0	0	0
All	All	7083	0	6353	200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (200) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:HG22	6:A:317:HOH:O	1.69	0.93
1:A:82:ASN:HD21	1:A:118:ARG:HH11	0.96	0.92
3:H:383:LYS:H	3:H:383:LYS:HD2	1.34	0.90
4:I:11:DC:H1'	4:I:12:DC:H5"	1.59	0.82
1:A:87:ILE:HD12	1:A:87:ILE:O	1.81	0.81
1:A:82:ASN:ND2	1:A:118:ARG:HH11	1.79	0.79
2:B:60:THR:HG23	2:B:62:THR:H	1.48	0.78
1:A:82:ASN:HD21	1:A:118:ARG:NH1	1.79	0.77
1:F:161:THR:HG21	1:F:163:HIS:CE1	2.23	0.74
2:B:8:GLN:HE21	2:B:107:CYS:H	1.38	0.72
2:B:82:SER:HB2	2:B:85:TYR:HB2	1.72	0.71
4:D:10:DT:H2"	4:D:11:DC:H5'	1.73	0.71
2:B:108:VAL:HG11	2:B:125:LEU:HB3	1.74	0.70
2:B:136:ASP:HA	2:B:139:ALA:HB3	1.74	0.69
3:C:383:LYS:HB3	3:C:383:LYS:NZ	2.07	0.69
4:I:14:DC:H2"	4:I:15:DT:H5'	1.75	0.68
2:G:71:ALA:HB3	2:G:131:ARG:HH22	1.60	0.66
3:H:382:PRO:HB2	3:H:383:LYS:HD2	1.78	0.65
3:C:364:LYS:HB2	3:C:411:VAL:HG22	1.78	0.65
2:G:39:GLU:O	2:G:42:THR:HG22	1.97	0.64
2:B:108:VAL:HG12	2:B:109:ILE:N	2.13	0.64
2:G:91:GLU:HG3	2:G:92:ALA:H	1.61	0.64
2:G:60:THR:HG23	2:G:62:THR:H	1.63	0.63
1:F:79:TRP:CZ2	1:F:86:PRO:HD3	2.35	0.62
4:D:11:DC:H2"	4:D:12:DC:C5'	2.30	0.61
2:G:71:ALA:HB3	2:G:131:ARG:NH2	2.15	0.61
2:G:70:PRO:O	2:G:71:ALA:HB3	2.00	0.61
1:A:70:PHE:CE2	1:A:152:VAL:HG21	2.36	0.61
3:H:345:LEU:HD22	3:H:356:TRP:NE1	2.15	0.60
1:A:97:VAL:H	1:A:127:GLN:HE22	1.49	0.60
2:B:106:VAL:O	2:B:108:VAL:HG23	2.02	0.60
2:G:16:GLU:OE2	2:G:20:LYS:HB2	2.01	0.59
2:G:8:GLN:HE21	2:G:107:CYS:H	1.51	0.59
2:B:137:ALA:O	2:B:140:GLN:HG3	2.02	0.59
2:B:5:VAL:HG12	2:B:105:GLY:O	2.02	0.59
3:H:383:LYS:N	3:H:383:LYS:HD2	2.12	0.59
3:H:353:PHE:CD2	3:H:370:GLU:HG2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:VAL:HG12	2:B:109:ILE:H	1.67	0.58
2:G:86:VAL:O	2:G:86:VAL:HG13	2.04	0.58
2:B:138:LEU:H	2:B:138:LEU:HD12	1.70	0.57
2:G:108:VAL:HG12	2:G:109:ILE:N	2.19	0.57
2:G:9:ARG:O	2:G:13:GLU:HG2	2.04	0.57
4:D:11:DC:C2'	4:D:12:DC:H5"	2.35	0.56
3:H:335:ILE:HD12	3:H:339:GLN:HE21	1.70	0.56
2:B:93:GLY:O	2:B:116:LEU:HB2	2.06	0.56
3:H:389:LEU:HD23	3:H:389:LEU:O	2.05	0.56
1:F:63:VAL:HB	1:F:74:VAL:HG22	1.88	0.56
1:F:114:SER:HB3	2:G:33:ARG:HH12	1.71	0.56
4:D:13:DT:H2"	4:D:14:DC:H5'	1.87	0.56
4:D:11:DC:H2"	4:D:12:DC:H5"	1.88	0.56
2:B:131:ARG:O	2:B:135:GLU:HB2	2.06	0.55
4:I:9:DA:H1'	4:I:10:DT:H5"	1.87	0.55
2:B:81:PRO:HB2	2:B:86:VAL:HG11	1.88	0.55
3:C:345:LEU:HD21	3:C:354:ILE:HG12	1.87	0.55
3:H:356:TRP:HZ3	3:H:361:TRP:HE3	1.55	0.55
1:A:126:ASN:O	1:A:127:GLN:HB2	2.05	0.55
3:H:417:ASP:OD1	3:H:420:SER:HB3	2.07	0.55
2:G:87:ASP:HB3	2:G:96:TYR:HB2	1.89	0.54
2:B:83:ARG:HG3	2:B:84:GLU:H	1.72	0.54
3:H:345:LEU:HD13	3:H:356:TRP:CZ2	2.42	0.54
1:F:130:ARG:HH12	1:F:132:ASN:HD22	1.54	0.54
2:B:115:ASP:OD1	2:B:118:ARG:HD3	2.08	0.54
2:G:118:ARG:HB3	2:G:120:ASP:OD1	2.08	0.53
2:B:32:PHE:N	2:B:32:PHE:CD2	2.76	0.53
2:B:83:ARG:HG3	2:B:84:GLU:OE2	2.08	0.53
3:H:345:LEU:HD22	3:H:356:TRP:CD1	2.44	0.53
4:I:13:DT:H1'	4:I:14:DC:H5"	1.90	0.53
4:D:11:DC:H1'	4:D:12:DC:H5"	1.90	0.53
3:H:342:LEU:HD23	3:H:342:LEU:O	2.08	0.53
5:E:15:DC:H2'	5:J:1:DA:O4'	2.09	0.52
3:C:417:ASP:O	3:C:421:LEU:HD23	2.08	0.52
2:G:68:PHE:CE1	2:G:97:LEU:HB3	2.44	0.52
3:H:383:LYS:CD	3:H:383:LYS:H	2.16	0.52
3:C:428:GLU:O	3:C:432:MET:HG3	2.09	0.52
3:C:379:LYS:NZ	4:D:9:DA:OP1	2.43	0.52
2:B:23:ARG:HD2	2:B:25:CYS:HB3	1.91	0.52
1:A:74:VAL:O	1:A:87:ILE:HD11	2.09	0.52
1:A:87:ILE:HG13	6:A:310:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:TRP:C	2:B:114:ILE:HD12	2.31	0.51
4:I:14:DC:H2"	4:I:15:DT:C5'	2.40	0.51
3:C:373:ARG:HG3	3:C:373:ARG:HH11	1.76	0.51
2:G:27:ILE:HB	2:G:55:ILE:CG2	2.40	0.51
3:H:367:ASP:O	3:H:370:GLU:HB3	2.11	0.51
2:G:118:ARG:HH11	2:G:118:ARG:HB2	1.75	0.50
2:B:68:PHE:CZ	2:B:97:LEU:HD13	2.46	0.50
3:H:393:LEU:HA	3:H:396:TYR:HD2	1.76	0.50
2:B:8:GLN:NE2	2:B:107:CYS:H	2.08	0.50
4:D:1:DG:O4'	4:I:15:DT:H2'	2.12	0.50
2:G:97:LEU:HB2	2:G:110:TRP:HZ3	1.77	0.50
1:A:66:ASP:OD2	1:A:163:HIS:CD2	2.65	0.49
2:B:14:ASN:N	2:B:14:ASN:HD22	2.09	0.49
2:B:70:PRO:O	2:B:71:ALA:HB2	2.11	0.49
4:D:5:DC:H2"	4:D:6:DC:H5"	1.94	0.49
2:B:57:PHE:HB2	2:B:60:THR:HG22	1.94	0.49
2:B:138:LEU:N	2:B:138:LEU:HD12	2.28	0.49
2:G:20:LYS:HG3	2:G:20:LYS:O	2.11	0.49
1:A:144:LYS:HE3	3:H:407:GLY:CA	2.43	0.49
3:H:385:ASN:OD1	3:H:387:GLU:HB2	2.13	0.49
1:A:113:TYR:CE2	2:B:28:LYS:HD2	2.48	0.48
2:B:95:VAL:CG2	2:B:116:LEU:HG	2.43	0.48
1:A:144:LYS:HE3	3:H:407:GLY:HA3	1.95	0.48
3:H:362:GLU:HG3	3:H:413:ARG:HB3	1.95	0.48
2:G:28:LYS:HG3	2:G:58:VAL:HG21	1.94	0.48
2:G:91:GLU:HB3	2:G:94:LYS:HG2	1.95	0.47
3:C:383:LYS:HB3	3:C:383:LYS:HZ2	1.79	0.47
1:F:114:SER:HB3	2:G:33:ARG:NH1	2.29	0.47
4:D:5:DC:H2"	4:D:6:DC:C5'	2.44	0.47
3:H:409:ARG:HG2	3:H:410:TYR:CE2	2.49	0.47
3:C:326:LEU:O	3:C:421:LEU:HD12	2.14	0.47
1:A:87:ILE:HD12	1:A:87:ILE:C	2.34	0.47
2:G:89:GLU:O	2:G:90:ARG:C	2.53	0.47
1:A:103:VAL:HG21	1:A:129:ALA:HB2	1.96	0.47
3:C:379:LYS:HE3	6:D:107:HOH:O	2.15	0.47
3:H:336:GLN:H	3:H:339:GLN:NE2	2.13	0.47
2:G:10:SER:O	2:G:14:ASN:HB2	2.15	0.47
2:G:108:VAL:CG1	2:G:109:ILE:N	2.79	0.46
1:A:104:THR:HB	1:A:153:PHE:HE1	1.79	0.46
2:B:88:LEU:HD23	2:B:95:VAL:HG22	1.98	0.46
2:G:89:GLU:O	2:G:91:GLU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LYS:HE3	2:B:58:VAL:HG21	1.96	0.46
3:C:383:LYS:HB3	3:C:383:LYS:HZ3	1.81	0.46
1:F:63:VAL:HG22	1:F:64:ARG:N	2.30	0.46
1:F:115:ALA:HB2	1:F:146:PHE:CZ	2.49	0.46
2:G:68:PHE:CZ	2:G:97:LEU:HD13	2.50	0.46
2:G:28:LYS:HG3	2:G:58:VAL:CG2	2.46	0.46
1:F:112:ASN:HD22	1:F:112:ASN:C	2.19	0.45
2:B:88:LEU:CD2	2:B:95:VAL:HG22	2.47	0.45
2:B:115:ASP:O	2:B:117:HIS:N	2.49	0.45
3:H:335:ILE:O	3:H:335:ILE:HG23	2.16	0.45
1:F:64:ARG:HG3	6:F:302:HOH:O	2.16	0.45
1:A:106:MET:HE1	2:B:65:SER:N	2.32	0.45
1:F:161:THR:HG22	1:F:162:TYR:N	2.30	0.45
4:D:10:DT:C2'	4:D:11:DC:H5'	2.45	0.45
2:B:84:GLU:HG2	2:B:84:GLU:O	2.18	0.44
2:G:14:ASN:HD22	2:G:14:ASN:HA	1.65	0.44
2:B:95:VAL:HG21	2:B:116:LEU:HG	1.98	0.44
4:D:9:DA:H2"	4:D:10:DT:H5'	2.00	0.44
4:D:11:DC:H2"	4:D:12:DC:H5'	1.98	0.44
3:H:368:PRO:C	3:H:370:GLU:H	2.20	0.44
2:G:63:ASN:N	2:G:63:ASN:HD22	2.16	0.44
2:B:98:LYS:HA	2:B:110:TRP:O	2.18	0.44
1:A:87:ILE:O	1:A:87:ILE:CD1	2.59	0.44
3:C:361:TRP:HB3	3:C:414:PHE:HB2	2.00	0.44
1:A:70:PHE:CZ	1:A:152:VAL:HG21	2.53	0.43
3:H:389:LEU:HD23	3:H:389:LEU:C	2.37	0.43
1:A:148:LEU:HB2	1:A:162:TYR:HB3	2.00	0.43
3:H:348:LYS:HG2	3:H:348:LYS:H	1.67	0.43
1:A:111:GLU:HG3	1:A:144:LYS:NZ	2.34	0.43
2:B:108:VAL:CG1	2:B:109:ILE:N	2.81	0.43
3:H:350:CYS:HA	3:H:353:PHE:CE1	2.53	0.43
2:B:27:ILE:HD13	2:B:114:ILE:HD11	1.99	0.43
2:B:109:ILE:HD11	2:B:128:ASP:OD2	2.18	0.43
2:G:60:THR:CG2	2:G:62:THR:OG1	2.66	0.43
2:G:134:GLN:O	2:G:138:LEU:HG	2.18	0.43
3:H:338:TRP:CE2	3:H:339:GLN:HG3	2.54	0.43
3:C:359:ASP:OD2	3:C:359:ASP:C	2.57	0.43
4:D:5:DC:C2'	4:D:6:DC:H5"	2.49	0.43
3:H:345:LEU:HB3	3:H:356:TRP:NE1	2.33	0.42
1:A:113:TYR:CZ	2:B:28:LYS:HD2	2.53	0.42
2:B:63:ASN:HD22	2:B:63:ASN:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:70:PRO:O	2:G:71:ALA:CB	2.67	0.42
1:F:79:TRP:CH2	1:F:86:PRO:HD3	2.55	0.42
1:A:126:ASN:O	1:A:127:GLN:CB	2.68	0.42
3:H:341:LEU:HD21	3:H:371:VAL:HG11	2.00	0.42
3:C:342:LEU:HA	3:C:342:LEU:HD12	1.90	0.42
2:B:86:VAL:HG13	2:B:86:VAL:O	2.20	0.42
2:B:28:LYS:O	2:B:55:ILE:HA	2.19	0.42
2:G:32:PHE:HB3	2:G:35:ARG:HG3	2.02	0.42
3:C:321:ILE:HB	3:C:322:PRO:HD2	2.01	0.42
4:I:8:DC:OP1	4:I:8:DC:H4'	2.19	0.41
2:G:27:ILE:CD1	2:G:114:ILE:HD11	2.50	0.41
2:G:3:ARG:HD3	2:G:135:GLU:OE2	2.20	0.41
3:H:350:CYS:HA	3:H:353:PHE:HE1	1.85	0.41
1:A:60:GLY:O	1:A:61:GLU:HB3	2.21	0.41
2:G:21:LEU:HD21	2:G:60:THR:HG21	2.02	0.41
2:B:131:ARG:HA	2:B:134:GLN:HG2	2.03	0.41
3:C:354:ILE:HG13	3:C:365:LEU:HD23	2.02	0.41
2:G:90:ARG:HE	2:G:90:ARG:HB2	1.77	0.41
3:C:320:VAL:HG12	3:C:321:ILE:HG23	2.03	0.41
3:C:379:LYS:O	3:C:380:ASN:HB3	2.20	0.41
2:G:3:ARG:HH11	2:G:135:GLU:CD	2.24	0.41
3:C:389:LEU:HD23	3:C:389:LEU:C	2.41	0.41
2:B:21:LEU:HD22	2:B:57:PHE:CD1	2.56	0.41
4:D:11:DC:C1'	4:D:12:DC:H5"	2.50	0.41
2:G:108:VAL:HG13	2:G:126:GLU:O	2.21	0.41
3:H:362:GLU:HA	3:H:413:ARG:CB	2.51	0.41
2:B:108:VAL:CG1	2:B:125:LEU:HB3	2.48	0.41
2:G:91:GLU:HB3	2:G:94:LYS:CG	2.51	0.41
3:H:356:TRP:HZ3	3:H:361:TRP:CE3	2.35	0.41
3:C:378:ARG:HG3	3:C:378:ARG:O	2.21	0.41
1:A:139:ARG:HD3	1:A:139:ARG:N	2.36	0.41
2:G:55:ILE:HD13	2:G:66:LEU:HD12	2.03	0.40
3:H:340:PHE:CE2	3:H:375:TRP:HB2	2.56	0.40
3:H:345:LEU:HB3	3:H:356:TRP:CZ2	2.56	0.40
3:H:362:GLU:HA	3:H:413:ARG:HB3	2.04	0.40
2:B:55:ILE:CG2	2:B:56:ALA:N	2.84	0.40
1:A:149:THR:HG21	2:B:63:ASN:O	2.21	0.40
3:H:341:LEU:CD2	3:H:371:VAL:HG11	2.52	0.40
3:H:337:LEU:HA	3:H:375:TRP:CZ3	2.57	0.40
3:H:378:ARG:HH11	3:H:378:ARG:HG3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	117/204 (57%)	112 (96%)	5 (4%)	0	100 100
1	F	116/204 (57%)	111 (96%)	5 (4%)	0	100 100
2	B	127/142 (89%)	111 (87%)	12 (9%)	4 (3%)	5 3
2	G	126/142 (89%)	106 (84%)	14 (11%)	6 (5%)	3 1
3	C	116/166 (70%)	112 (97%)	4 (3%)	0	100 100
3	H	91/166 (55%)	65 (71%)	21 (23%)	5 (6%)	2 0
All	All	693/1024 (68%)	617 (89%)	61 (9%)	15 (2%)	8 5

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	81	PRO
2	G	58	VAL
3	H	335	ILE
2	B	116	LEU
2	G	24	GLU
2	G	82	SER
2	G	90	ARG
2	B	91	GLU
2	G	14	ASN
3	H	382	PRO
2	G	130	GLU
3	H	383	LYS
2	B	58	VAL
3	H	334	PRO
3	H	366	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/179 (56%)	95 (95%)	5 (5%)	30	37
1	F	100/179 (56%)	96 (96%)	4 (4%)	38	49
2	B	114/123 (93%)	102 (90%)	12 (10%)	8	8
2	G	113/123 (92%)	103 (91%)	10 (9%)	12	12
3	C	102/145 (70%)	98 (96%)	4 (4%)	39	51
3	H	84/145 (58%)	79 (94%)	5 (6%)	24	28
All	All	613/894 (69%)	573 (94%)	40 (6%)	21	24

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	THR
1	A	112	ASN
1	A	139	ARG
1	A	155	ASN
1	A	175	GLU
2	B	23	ARG
2	B	25	CYS
2	B	48	CYS
2	B	55	ILE
2	B	63	ASN
2	B	87	ASP
2	B	94	LYS
2	B	98	LYS
2	B	103	LEU
2	B	116	LEU
2	B	124	CYS
2	B	129	GLU
3	C	330	THR
3	C	379	LYS
3	C	383	LYS
3	C	436	LYS
1	F	87	ILE

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Mol	Chain	Res	Type
1	F	110	ASP
1	F	112	ASN
1	F	162	TYR
2	G	14	ASN
2	G	23	ARG
2	G	38	GLU
2	G	67	GLN
2	G	82	SER
2	G	91	GLU
2	G	103	LEU
2	G	117	HIS
2	G	118	ARG
2	G	140	GLN
3	H	369	ASP
3	H	383	LYS
3	H	398	ASP
3	H	408	LYS
3	H	419	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	112	ASN
1	A	119	ASN
1	A	127	GLN
1	A	163	HIS
2	B	8	GLN
2	B	14	ASN
2	B	41	GLN
2	B	134	GLN
2	B	140	GLN
3	C	380	ASN
1	F	112	ASN
1	F	127	GLN
1	F	132	ASN
2	G	8	GLN
2	G	14	ASN
2	G	41	GLN
3	H	339	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	119/204 (58%)	0.60	3 (2%) 61 73	42, 58, 84, 96	0
1	F	118/204 (57%)	0.52	2 (1%) 73 83	37, 51, 71, 94	0
2	B	131/142 (92%)	1.26	25 (19%) 2 3	60, 85, 115, 126	0
2	G	130/142 (91%)	0.99	18 (13%) 4 8	56, 77, 107, 119	0
3	C	118/166 (71%)	0.42	2 (1%) 73 83	39, 59, 83, 89	0
3	H	93/166 (56%)	2.20	43 (46%) 0 0	62, 112, 139, 146	0
4	D	15/15 (100%)	-0.06	0 100 100	46, 52, 62, 63	0
4	I	15/15 (100%)	0.04	0 100 100	49, 62, 77, 77	0
5	E	15/15 (100%)	-0.09	0 100 100	43, 49, 60, 65	0
5	J	15/15 (100%)	-0.01	0 100 100	47, 57, 71, 73	0
All	All	769/1084 (70%)	0.88	93 (12%) 6 10	37, 67, 119, 146	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	421	LEU	9.4
2	B	138	LEU	7.9
3	H	360	GLY	7.7
2	B	137	ALA	6.0
3	H	422	LEU	5.8
3	H	356	TRP	5.7
3	H	345	LEU	5.6
3	H	353	PHE	5.5
2	B	93	GLY	5.4
3	H	424	TYR	5.4
2	B	92	ALA	5.4
3	H	350	CYS	5.2
2	G	140	GLN	5.1

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Mol	Chain	Res	Type	RSRZ
3	H	419	GLN	4.3
3	H	365	LEU	4.3
3	H	373	ARG	4.1
3	H	423	GLY	4.1
2	B	71	ALA	4.1
2	G	139	ALA	3.9
3	H	372	ALA	3.8
3	H	364	LYS	3.8
2	G	82	SER	3.7
3	H	414	PHE	3.7
3	H	341	LEU	3.6
3	H	351	GLN	3.6
2	B	70	PRO	3.6
3	H	358	GLY	3.6
2	G	81	PRO	3.5
2	B	14	ASN	3.5
2	G	133	GLN	3.5
2	G	7	ASP	3.5
3	H	361	TRP	3.5
3	H	420	SER	3.4
3	H	417	ASP	3.3
3	H	354	ILE	3.3
2	B	140	GLN	3.3
3	H	416	CYS	3.3
3	H	348	LYS	3.2
2	B	10	SER	3.2
3	H	405	THR	3.1
1	A	64	ARG	3.0
2	G	83	ARG	3.0
2	B	139	ALA	3.0
3	H	384	MET	3.0
2	B	5	VAL	3.0
2	G	127	PHE	3.0
3	H	401	ILE	2.9
3	H	368	PRO	2.9
3	H	337	LEU	2.9
1	F	175	GLU	2.8
3	H	338	TRP	2.8
2	B	82	SER	2.7
3	C	332	SER	2.7
2	B	83	ARG	2.7
2	B	116	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	330	THR	2.7
3	H	335	ILE	2.6
2	B	94	LYS	2.6
3	H	383	LYS	2.6
3	H	355	SER	2.6
2	B	109	ILE	2.6
2	B	86	VAL	2.5
3	H	415	VAL	2.5
2	G	87	ASP	2.5
2	G	38	GLU	2.5
1	A	178	ARG	2.4
2	G	90	ARG	2.4
2	B	105	GLY	2.3
2	G	138	LEU	2.3
3	H	343	GLU	2.3
2	B	133	GLN	2.3
2	G	126	GLU	2.3
3	H	413	ARG	2.3
2	G	86	VAL	2.3
3	H	377	LYS	2.3
2	G	117	HIS	2.3
3	H	374	ARG	2.2
3	H	349	SER	2.2
1	F	177	ARG	2.2
3	H	402	ILE	2.1
3	H	407	GLY	2.1
3	H	375	TRP	2.1
2	G	116	LEU	2.1
3	H	346	THR	2.1
2	B	117	HIS	2.1
2	B	21	LEU	2.1
2	B	118	ARG	2.1
2	B	23	ARG	2.1
2	B	20	LYS	2.1
1	A	105	VAL	2.1
2	G	33	ARG	2.0
2	G	136	ASP	2.0
2	B	55	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.